(12)

ONR PUBLICATIONS/PATENTS/PRESENTATIONS/HONORS REPORT
1 October 1992 through 30 September 1993

R&T Number: 4113641---02

Contract/Grant Number: N00014-89-J-1644

Contract/Grant Title: Studies in Nonlinear Numerical Analysis

Principal Investigator: Donald J. Rose

Mailing Address: Department of Computer Science
Duke University
Box 90129
Durham, NC 27708-0129

Phone Number: 919-660-6544 E-Mail Address: djr@cs.duke.edu

a. Number of Papers Submitted to Refereed Journals but not yet published: 1

An Analysis of Approximate Nonlinear Elimination, TR-1993-21, DUKE CS DEPT; submitted to *SIAM Journal on Scientific Computing*; with Paul J. Lanzkron.

b. Number of Papers Published in Refereed Journals: 1

Linear Algebraic Transformations of the Bidomain Equations and Their Implications on Numerical Methods, *Mathematical Biosciences*; with N. Hooke, C. Henriquez, and P. Lanzkron.

c. Number of Books/Chapters Submitted but not yet Published: 0

d. Number of Books or Chapters Published: 0

e. Number of Technical Reports & Non-Refereed Papers:

(Papers submitted to journals are also department technical reports.)

f. Number of Patents Filed: 0

g. Number of Patents Granted: 0

h. Number of Invited Presentations at Workshops or Professional Society Meetings: 0

i. Number of Contributed Presentations at Workshops or Professional Society Meetings: 1

1993 Householder Symposium on Numerical Analysis
June 12 - 18, 1993; Los Angeles, CA

j. Honors/Awards/Prizes for Contract/Grant Employees:

k. Number of Full Time Equivalent Graduate Students and Post-Docs Supported This Year Under This Grant: Graduate Students: 3
Post-Docs: 0

Of these:
FTE Female Graduate Students: 1
FTE Minority Graduate Students: 0
FTE Female Post-Docs: 0
FTE Minority Post-Docs: 0

k 1 undergraduates:
1 male, 1 female

DUKE UNIVERSITY DEPARTMENT OF COMPUTER SCIENCE

246 North Building
Box 90129
Durham, NC 27708-0129
(919) 660-6544

August 19, 1993

Dr. Richard Lau
Office of Naval Research
Math Science Division Code 1111
800 North Quincey Street
Arlington, VA 22217

Dear Dr. Lau:

This communication serves as the progress report you requested by phone earlier this week.

I have been working intensively on the quantum optimal control (QOC) problem as formulated by H. Rabitz. ONR also supports my Ph.D. student, Li-Ling Huang, in this work. We have devised a complete algorithmic strategy, capable of higher order convergence, and have implemented this strategy in a prototype code. This problem is an optimal control problem and involves many areas of numerical analysis. We have devised or tuned for this problem special implicit ODE solvers, nonlinear equation solvers and linear iterative methods.

The next step in the QOC problem is to resolve 1D and 2D problems in space to get a more realistic assessment of our algorithmic strategy than the simple problems we have solved can provide. Rabitz has solved these problems previously by the currently used methodology. We will then refine and redesign our approach with a view to providing a tool for the appropriate scientific community. A version of this software environment will be specialized to run on our CM5, and we will assess the applicability of this parallel computing platform for such problems.

I am working with another student, Scott Bigham, on automatic differentiation. Bigham is funded by my ASSERT funding. This study arises as part of my long term goal to produce a nonlinear equations solver that is robust, accurate, and has good convergence properties.

Such an algorithm must employ a Newton-like strategy and hence requires computing the Jacobian. In many applications the Jacobian is computed analytically, then called as a function. Often there are errors if the original vector function is complicated. Automatic differentiation attempts to overcome some of these difficulties.

I continue to work on some aspects of linear iterative methods. I have recently formulated an approach I call IBI, Intersecting Block Iteration, which can be viewed as a general algebraic methodology with roots and motivation from "Domain Decomposition."

I had a very productive summer. Last Spring I began seeking an approach to organizing my summer research effort to have both an educational component and a research component. I decided finally on a working lunch seminar which met Tuesday, Wednesday and Thursday from 12 - 2 pm. My ONR supported research team and a few additional students from my Spring graduate numerical analysis course attended. Included also were two undergraduates, both supported by ONR, one by my ASSERT award. We all spoke regularly giving approximately weekly progress reports. This kept me in tune with my students and allowed "instant feed back".

I was particularly pleased with the undergraduates. When I wrote my ASSERT proposal and asked for undergraduate funding, I frankly was unsure whether they would really be able to contribute. The seminar approach definitely helped here, as well as my idea to assign each undergrad a graduate student "mentor". This eliminated the intimidation factor from a senior faculty member to an undergrad, and, eventually, they felt at ease in their presentations.

Sincerely,

Donald J. Rose
Professor

DJR/gs